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NUMERICAL ANALYSIS OF LARGE EDDY SIMULATION

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Abstract. We have focused upon the development and validation of finite element methods for LES of turbulent flows in settings in which interaction with (possibly geometrically complex) boundaries are important. New results are presented in Section 2 on closure and convolution on bounded domains. Similarly, new near wall models were required; our method for developing these is described and one from our work is presented in Section 3. The difficulties in closure and wall modelling suggest a second approach: direct simulation of large eddy motion. We give an extension of this approach to nonlinear, equilibrium flows - a step closer to turbulence for an approach not requiring wall models or closure models.

1. Introduction

There is a natural interplay between Finite Element CFD and LES for topics such as: closure models, near wall models, and FEM postprocessing by

local averaging. Because of their geometric flexibility *and* their flexibility with respect to continuum models and linear or nonlinear boundary conditions, FEM's are a natural discretization in the LES of flows with complex boundaries. Adaptivity, highly developed for FEM's, has interesting potential for LES without modelling error. For example, using extensions of work in (John and Layton, 2001) reported in Section 4, a CFD mesh can be designed so that local averages of an inaccurate approximate flow field approximate the true local velocity averages with assured accuracy.

This paper surveys some of our work developing a mathematical foundation for finite element LES and presents some new results and extensions of this work. Many of the reports cited herein are available at <http://www.math.pitt.edu/~wj1>.

Consider therefore the turbulent flow of an incompressible fluid in three dimensions, bounded by walls and driven by a body force $f(x, t)$. The velocity-pressure (u, p) satisfy the Navier Stokes equations, given by:

$$u_t + \operatorname{div}(uu) - 2Re^{-1} \operatorname{div}(\mathbb{D}(u)) + \operatorname{grad} p = f(x, t), \text{ and } \operatorname{div} u = 0, \quad (1)$$

in a domain Ω complemented by boundary and initial conditions

$$u = 0 \text{ on walls, and } u(x, 0) = u_0(x),$$

where $\mathbb{D}(u) = (\operatorname{grad} u + \operatorname{grad} u^t)/2$ is the velocity deformation tensor. Picking a length scale δ and an associated averaging kernel $g_\delta(x) := \delta^{-3}g(x/\delta)$, where $g(x)$ is a mollifier satisfying certain properties, local velocity and pressure averages are frequently defined by convolution with $g(x)$, $\bar{u} := g_\delta * u$, $\bar{p} := g_\delta * p$, etc., where all functions are, when necessary, extended by 0 off the flow domain to compute the required average.

For compactness, we will only discuss herein the case of constant averaging radius δ . Alternate approaches include a variational definition of the large eddies (Layton, 1999), (Hughes *et al.*, 2001), and differential filters, introduced by Germano in the 1980's, wherein (in effect) $\delta = \delta(x) \rightarrow 0$ as x approaches walls in a manner intrinsic to the NSE and the domain's geometry, (Layton and Lewandowski, 2001).

2. Convolution on Bounded Domains and Closure

With constant averaging radius, δ , convolution operators commute with differential operators *in the absence of boundaries*. With boundaries, extra terms arise which are often overlooked. For example, filtering (1) with $g_\delta(x)$ on a bounded domain gives the following space filtered equations for $\bar{u} := g_\delta * u$, $\bar{p} := g_\delta * p$ (see (Dunca *et al.*, 2001))

$$\bar{u}_t + \operatorname{div}(\bar{u} \bar{u}) - 2Re^{-1} \operatorname{div}(\mathbb{D}(\bar{u})) + \operatorname{grad} \bar{p} + \operatorname{div}(\mathbb{T}(u)) = \bar{f} + A_\delta(\sigma), \quad (2)$$

where σ is the stress of the unknown flow and $\mathbb{T}(u) := \overline{uu} - \bar{u} \bar{u}$ is the Reynolds stress tensor. A direct calculation in (Dunca *et al.*, 2001) using the theory of distributions reveals that

$$A_\delta(\sigma) := \int_{\partial\Omega} g_\delta(x-s)(\sigma \cdot \hat{n})(s)ds, \quad \sigma := 2Re^{-1}\mathbb{D}(u) - pI,$$

which can be interpreted as a boundary stress distribution smeared out onto the entire flow domain. Since the $A_\delta(\sigma)$ term in (2) is normally neglected, it might be hoped to be negligible. Unfortunately, this is not the case, as is seen in the following result, (Dunca *et al.*, 2001).

Proposition. *Let $\|w\|_{L^p} := (\int_{\mathbb{R}^3} |w|^p dx)^{1/p}$, $1 \leq p < \infty$ denote the usual L^p norm, $1 \leq p < \infty$ and $\|w\|_{L^\infty} := \text{ess sup}_{x \in \mathbb{R}^3} |w|$. Then for $1 \leq p \leq \infty$*

$$\|A_\delta\|_{L^p} \rightarrow 0 \text{ as } \delta \rightarrow 0.$$

if and only if the normal stress is identically zero on the boundary of the flow domain

$$\sigma \cdot \hat{n} \equiv 0 \text{ on the boundary. } \square$$

The proof of this result is moderately technical but the importance of the result is clear: *the term $A_\delta(\sigma)$ cannot be omitted if the boundary influences the flow!*

It is well-known that (2) are *not closed* for periodic problems due (only) to the Reynolds stress tensor $\mathbb{T}(u)$ and numerous LES models have been developed to model $\mathbb{T}(u)$, see, e.g., (Iliescu and Layton, 1998), (Berselli *et al.*, 2001), (Layton, 2000), (Galdi and Layton, 1999), (Layton and Lewandowski, 2001) for our work on closure. For flows with real walls or other boundaries, (2) are not closed due to both $\mathbb{T}(u)$ and the “smeared” wall stress operator $A_\delta(\sigma)$. More detailed understanding of $A_\delta(\sigma)$ is necessary to model correctly the interaction of large eddies with walls; see (Dunca *et al.*, 2001) for first steps.

3. Near Wall Models: Boundary Conditions for LES

Either modeling or omitting the smeared wall stress term $A_\delta(\cdot)$, boundary conditions are still required for the large eddies \bar{u} and simply imposing $\bar{u} = 0$ at walls is inconsistent, see (Galdi and Layton, 1999), Figure 1. This inconsistency is intuitively clear: a tornado, as an example of a large eddy, does move/slip along the ground.

What are then the correct boundary conditions? Motivated by this example of a tornado, we have explored no-penetration and slip-with-friction conditions (see, e.g., (Navier, 1823) and (Maxwell, 1879) for antecedents) for \bar{u} :

$$\bar{u} \cdot \hat{n} = 0 \text{ and } \beta_j \bar{u} \cdot \hat{\tau}_j + t(\bar{u}) \cdot \hat{\tau}_j = 0 \text{ on walls,} \quad (3)$$

where \hat{n}, τ_1, τ_2 are unit normal and tangent vectors to the wall (Layton, 2001), and t is the Cauchy stress or traction vector. The effective friction coefficient β for the large eddies is calculated explicitly in (Sahin, 2000) and (John *et al.*, 2001)

$$\beta = \beta(\delta, Re) \text{ or } \beta = \beta(\delta, |\bar{u} \cdot \hat{\tau}_j|) : \text{ large eddy friction coefficient.}$$

The conditions (3) thus allow both linear and nonlinear near wall models. For turbulent channel flow, the linear model, based on a global Reynolds number, seems to suffice. However, for flows in complex geometries, the local Reynolds number, related to the slip velocity $|\bar{u} \cdot \hat{\tau}_j|$, varies greatly from recirculation zones to mean stream regions. Thus, the nonlinear model seems necessary.

The friction laws in (Sahin, 2000), (John *et al.*, 2001) are calculated using boundary layer theory, with different results for different types of turbulent layers. For example, for a power law layer the linear wall model's effective friction coefficient is as follows. Let $\Gamma[\cdot]$ denote the usual gamma function and $\Gamma[\cdot, \cdot]$ the incomplete gamma function, $\eta = 0.21Re^{-1}$ and $Z := \eta/\delta$

$$\beta(\delta, \eta) = \frac{Re^{-1} Z^{1/7} [7\Gamma[\frac{15}{14}] - \frac{1}{2}\Gamma[\frac{1}{14}, Z^2]]}{2\sqrt{\pi}\delta^2 [Z^{1/7} \{\Gamma[\frac{4}{7}] - \Gamma[\frac{4}{7}, Z^2]\} + \sqrt{\pi}(1 - \text{erf}(Z))]}.$$

A very good (and simple) approximation is given (to 4 decimal places) by the effective friction coefficient:

$$\beta(\delta, Re) \cong Re^{-1} \delta^{-2} 1.22e^{-0.008/Z}. \quad (4)$$

From this simple formula we see that:

- As $\delta \rightarrow 0$, for fixed Re , the friction $\beta \rightarrow \infty$, i.e., the boundary conditions (3) reduce to no slip.
- As $Re \rightarrow \infty$ for fixed δ , the friction coefficient $\beta \rightarrow 0$, i.e., the boundary conditions (3) reduce to free-slip and no-penetration, as appropriate for the Euler equations.

To explain the nonlinear friction laws we note that for a power law layer (and other profiles as well), the slip speed, $s := \sqrt{|\bar{u} \cdot \hat{\tau}_1|^2 + |\bar{u} \cdot \hat{\tau}_2|^2}$ is a monotone increasing function of Re for δ fixed. Expressing this as

$s = g(Re), g'(Re) > 0$ implies that the inverse function $g^*(\cdot)$ of $g(\cdot)$ exists. We can then write $Re = g^*(s)$. Inserting this inverted relation into (4) yields nonlinear friction laws:

$$\beta_j(\delta, g^*(|\bar{u} \cdot \hat{\tau}_j|)) \cong 1.22\delta^{-2} g^*(|u \cdot \hat{\tau}_j|) e^{-0.0090/g^*(|\bar{u} \cdot \hat{\tau}_j|)}.$$

This program can be carried out for different types of turbulent boundary layer profiles, see (John *et al.*, 2001) for detailed formulas.

4. Numerical Errors in LES

With closure models and boundary conditions selected, convergence of a chosen numerical method to the model's solution must be considered, e.g. (John and Layton, 2000), (Iliescu *et al.*, 2000), (Layton, 1996). For example, in (John and Layton, 2000) convergence for a FEM discretization of the Smagorinsky model is proven to be *uniform in Re*, as is often reported in practical simulations but hitherto unproven. This work does *not* address the modelling error itself however.

In recent work, we have devised new algorithms which give computable bounds on *both the modelling and the numerical errors*, (John and Layton, 2000). This work was begun in (John and Layton, 2001) for (linear) Stokes flow. Our current work, reported in this section, has extended those new methods to the (nonlinear) equilibrium NSE - a step closer to the true problem.

The approach is simple to describe: the fluid velocity is directly approximated and then postprocessed by local averaging, giving $g_\delta * u^h$ as an approximation to $\bar{u} = g_\delta * u$. One key is that the finite element mesh is adapted within the calculation so that $g_\delta * u^h$ approximates \bar{u} with assured accuracy, even when u^h is a bad approximation to u . The second key is that the averaging radius δ must be taken smaller than the local meshwidth of the refined mesh, $\delta \ll O(h)$. These new a posteriori estimators are given in (John and Layton, 2000) (and a new report in preparation). With these new estimators, the error is also concentrated in high frequencies and killed by postprocessing. Thus, the error in the large eddies is typically far smaller than the overall error, as in the following theorem.

Theorem. *Let the equilibrium NSE be solved by the FEM with finite element spaces satisfying the usual stability and local-polynomial degree k approximation conditions. Let the NSE solution be nonsingular with linearized dual H^{k+1} -regular. Then, the error in the large eddies $\|g_\delta * u^h - \bar{u}\|_{L^2}$ is related to (and much smaller than), the error in the velocity ($\|\nabla(u - u^h)\|$) and pressure ($\|p - p^h\|$) by, for any $\epsilon > 0$:*

$$\|g_\delta * u^h - \bar{u}\|_{L^2} \leq C \left\{ \left(Re^{-1} + \sqrt{h} \right) \left(\frac{k}{\delta} \right)^k \delta \|\nabla(u - u^h)\|_{L^2} \right.$$

$$\begin{aligned}
& + \left(\frac{h}{\delta}\right)^k \delta \left(\|p - p^h\|_{L^2} + \|\nabla \cdot (u - u^h)\|_{L^2} \right) \\
& + \left(\frac{h}{\delta}\right)^k \delta \left(\|\nabla(u - u^h)\|_{L^2}^2 + \delta^{\frac{1}{2}-\epsilon} \|u - u^h\|_{L^2}^2 \right) \}. \quad \square
\end{aligned}$$

This theorem also gives analytical guidance for relating δ and h . However, the related mesh-adaptation strategy is the most important practical contribution of this theory.

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